

# Optimal management and spatial patterns in a distributed shallow lake model

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## Abstract

We present a numerical framework to treat infinite time horizon spatially distributed optimal control problems via the associated canonical system derived by Pontryagin’s Maximum Principle. The basic idea is to consider the canonical system in two steps. First we perform a bifurcation analysis of canonical steady states using the continuation and bifurcation package `pde2path`, yielding a number of so called flat and patterned canonical steady states. In a second step we link `pde2path` to the two point boundary value problem solver `TOM` to study time dependent canonical system paths to steady states having the so called saddle point property. As an example we consider a shallow lake model with diffusion.

**Keywords:** Optimal Control, Pontryagin’s Maximum Principle, Bioeconomics, Canonical Steady States, Connecting Orbits

**MSC:** 49J20, 49N90, 35B32

## 1 Introduction

In [BX08] the authors consider economically motivated deterministic optimal control (OC) problems with an infinite time horizon and a continuum of spatial sites over which the state variable can diffuse. Using Pontryagin’s Maximum Principle (see §2.2 for general background and references on OC problems in a PDE setting) they derive the associated canonical system and show the remarkable result that under certain conditions on the Hamiltonian there occurs a Turing like bifurcation from flat to patterned steady states of the canonical system, and call this phenomenon optimal diffusion-induced instability (ODI). Here we present a numerical framework to (a) study such ODI bifurcations of canonical steady states (CSS) numerically in a simple way, and (b) study their optimality by calculating and evaluating time-dependent paths to and from such CSS. As an example we use one of the three examples presented in [BX08], namely a version of the, in the field of ecological economics, well-known shallow lake optimal control (SLOC) model, cf. [Sch98, MXdZ03, CB04].

We use the acronyms FCSS and PCSS for flat and patterned canonical steady states, and similarly FOSS and POSS for *optimal* canonical steady states, and summarize FOSS and POSS as OSS. The SLOC model has up to three (branches of) FCSS in relevant parameter regimes, and in these regimes we also find a large number of (branches of) PCSS. In this situation of multiple CSS a local stability analysis at a given CSS is in general not sufficient. Here, local stability analysis means that the stationary canonical system is analyzed, analogous to a steady-state analysis of the canonical system derived from an optimal control problem without spatial diffusion. It is well known and shown for many models that the appearance of multiple CSS (even if these steady-states are saddle-points) does not necessarily imply the appearance of multiple steady-states in the optimal system, cf. [GCF<sup>+</sup>08, KW10].

The reason is that there can exist a non-constant extremal solution, i.e. a canonical path connecting the state values of a given CSS to some other CSS, and yielding a higher objective value. Therefore, to study whether a CSS corresponds to an OSS, the values of the associated stable paths also have to be considered.

Here we numerically compute the bifurcation behavior of FCSS and PCSS for the SLOC model in some detail, and study their optimality by evaluation of their objective values  $J$  and comparison to time-dependent canonical paths. Such a global analysis is inevitable and has to accompany the local stability analysis. Since in general the pertinent ODEs or PDEs cannot be solved analytically we have to use numerical methods for the calculation of FCSS and in particular PCSS, and for the calculation of  $t$ -dependent canonical paths. For the steady state problem we use the continuation and bifurcation software `pde2path` [UWR14], based on a spatial finite element method (FEM) discretization, which we then combine with the boundary value problem (BVP) solver TOM to obtain canonical paths.

A standard reference on ecological economics or “Bioeconomics” is [Cla90], which also contains a very readable account, and applications, of Pontryagin’s Maximum Principle in the context of ODE models, while [GCF<sup>+</sup>08] focuses more on socio-economical ODE model applications. Besides in [BX08], and in [BX10], PDE models roughly similar to our diffusive SLOC model are considered in, e.g., [LW07, AAC11, DHM12, ACKLT13, ADS14], partly including numerical simulations. However, these works are in a finite time horizon setting, and with control constraints, which altogether gives a rather different setting from the one considered here. See Remark 2.4 for further comments.

In §2 we present the SLOC model. To give some background, in §2.1 we briefly present the 0D (ODE) version, and some basic concepts of optimal control, in particular Pontryagin’s Maximum Principle. In §2.2 we turn to the distributed case, explain the associated canonical system, and relate our method to other approaches to PDE OC problems. In §3 we explain the numerics to first compute the bifurcation diagram of canonical steady states, and then to solve the BVP in  $t$ . We mostly focus on one spatial dimension (1D), but also give a short outlook on the 2D case. It turns out that in the parameter regimes studied here the PCSS are not optimal, but nevertheless they play a relevant role. Moreover, calculating *optimal* canonical paths to FCSS yields interesting and to some extent counter-intuitive information about the optimal control of the distributed SLOC model.

In §4 we close with a short summary and discussion, and Appendix A contains remarks about the saddle point property for CSS in a PDE setting, starting on the discretized level.

Our software, including demo files and a manual to run some of the simulations in this paper, can be downloaded from [www.staff.uni-oldenburg.de/hannes.uecker/pde2path](http://www.staff.uni-oldenburg.de/hannes.uecker/pde2path). In fact, the present paper is the first in a series of four related works, the other three being [Uec15b, Gra15, Uec15a]: [Uec15b] contains a Quickstart guide and implementation details of the add on package `p2poc` to `pde2path` used for the computations in this paper. Thus, the reader interested in these details should read (parts of) [Uec15b] in parallel. Next, [Gra15] explains the usage of OCMat [orcos.tuwien.ac.at/research/ocmat\\_software/](http://orcos.tuwien.ac.at/research/ocmat_software/) to study 1D distributed OC problems based on spatial finite difference approximations, with the same SLOC model as in the present paper as an example, and thus obtaining comparable results, but also studying a second parameter regime. Finally, in [Uec15a] we apply `p2poc` to an OC problem for a reaction-diffusion *system* modeling a vegetation-water-grazing interaction. In contrast to the SLOC model studied here, this yields dominant patterned optimal steady states in wide parameter regimes, and thus interesting new results on spatial patterns in optimal harvesting.

## 2 The model, and background from optimal control

### 2.1 The shallow lake model without diffusion

A well known non-distributed or 0D version of the SLOC model, see e.g. [Wag03], can be formulated in dimensionless form as

$$V(P_0) := \max_{k(\cdot)} J(P_0, k(\cdot)), \quad J(P_0, k(\cdot)) := \int_0^\infty e^{-rt} J_c(P(t), k(t)) dt, \quad (1a)$$

$$\text{where } J_c(P, k) = \ln k - \gamma P^2 \quad (1b)$$

is the current value objective function, and  $P$  fulfills the ODE initial value problem

$$\dot{P}(t) = k(t) - bP(t) + \frac{P(t)^2}{1 + P(t)^2}, \quad P(0) = P_0 \geq 0. \quad (1c)$$

Here  $r, \gamma, b > 0$  are parameters,  $P = P(t)$  is the phosphorus contamination of the lake, which we want to keep low for ecological reasons, and  $k = k(t)$  is the phosphate load, for instance from fertilizers used by farmers, which farmers want high for economic reasons. The objective function consists of the concave increasing function  $\ln k$ , and the concave decreasing function  $-\gamma P^2$ ;  $b$  is the phosphorus degradation rate in the lake, and  $r$  is the discount rate. The discounted time integral in (1a) is typical for economic (or socio-political) problems, where “profits now” weight more than mid or far future profits. More specifically,  $r$  often corresponds to a long-term investment rate. We focus on the parameter choice

$$r = 0.03, \quad \gamma = 0.5, \quad b \in (0.5, 0.8) \text{ (primary bifurcation parameter)}, \quad (2)$$

and for the distributed case we shall additionally fix the diffusion parameter to  $D = 0.5$ .

The max in (1a) runs over all *admissible* controls  $k$  and (associated) states  $P$ ; for  $k$  we can take the space  $C_b^0([0, \infty), \mathbb{R})$ , and for  $P$  the space  $C_b^1([0, \infty), \mathbb{R})$ . In fact, we naturally have  $k(t) > 0$  for all  $t$  as  $J_c(k, P) \rightarrow -\infty$  as  $k \searrow 0$ , and then (1c) implies that  $P(t) > 0$  for all  $t > 0$ . On the other hand, see Remark 2.4 for comments on the case of state or control constraints.

By Pontryagin’s Maximum Principle [PBG62], see also, e.g., [GCF+08], an optimal solution  $(P^*(\cdot), k^*(\cdot))$  has to satisfy the first order optimality conditions

$$k^*(t) = \operatorname{argmax}_k \mathcal{H}(P(t), k, q(t), q_0) \quad \text{for almost all } t \geq 0, \quad (3a)$$

with the local current value Hamiltonian function

$$\mathcal{H}(P, k, q, q_0) := q_0 J_c(P, k) + q \left( k - bP + \frac{P^2}{1 + P^2} \right). \quad (3b)$$

The state  $P(\cdot)$  and costate  $q(\cdot)$  paths are solutions of the canonical system<sup>1</sup>

$$\dot{P}(t) = \partial_q \mathcal{H}(P(t), k^*(t), q(t)) = k^*(t) - bP(t) + \frac{P(t)^2}{1 + P(t)^2}, \quad (4a)$$

$$\dot{q}(t) = rq(t) - \partial_P \mathcal{H}(P(t), k^*(t), q(t)) = 2\gamma P(t) + q(t) \left( r + b - \frac{2P(t)}{(1 + P(t)^2)^2} \right), \quad (4b)$$

with

$$P(0) = P_0 > 0,$$

additionally satisfying the transversality condition

$$\lim_{t \rightarrow \infty} e^{-rt} q(t) = 0 \quad \text{if} \quad \liminf_{t \rightarrow \infty} P^*(t) > 0. \quad (5)$$

A solution  $(P(\cdot), q(\cdot))$  of the canonical system (4) is called a *canonical path*, and a steady state of (4) is called a *canonical steady state (CSS)*. Due to the strict concavity and continuous differentiability of the Hamiltonian function with respect to the control  $k$ , and the absence of control constraints, the solution of (3a) is given by

$$\partial_k \mathcal{H}(P(t), k(t), q(t)) = 0 \quad \text{which yields} \quad k^*(t) = -\frac{1}{q(t)}. \quad (6)$$

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<sup>1</sup>It can be proved that the problem is normal, i.e.  $q_0 > 0$ , and hence w.l.o.g.  $q_0 = 1$  can be assumed and is therefore subsequently omitted.

Consequently, for  $(P(\cdot), q(\cdot))$  a canonical path, i.e., a solution of the canonical system, with a slight abuse of notation we also call  $(P, k)$  with  $k = -1/q$  a canonical path. In particular, if  $(\hat{P}, \hat{q})$  is a CSS, so is  $(\hat{P}, \hat{k})$ . Canonical paths yield candidates for optimal solutions, defined as follows:

**Definition 2.1.**  $(P^*(\cdot), k^*(\cdot, P_0))$  is called an optimal solution of (1) if for every admissible  $k(\cdot)$  and associated  $P(\cdot)$  we have

$$J(P_0, k(\cdot)) \leq J(P_0, k^*(\cdot, P_0)) = V(P_0).$$

Then  $k^*(\cdot, P_0)$  is called an optimal control,  $P^*(\cdot)$  the corresponding optimal (state) path, and

$$\dot{P}(t) = k^*(t, P_0) - bP(t) + \frac{P(t)^2}{1 + P(t)^2} \quad (7)$$

is called the optimal ODE. A constant solution  $(P^*(\cdot), k^*(\cdot, P_0)) \equiv (\hat{P}, \hat{k}(\hat{P}))$  of (7) is called an optimal steady state (OSS).

It turns out that the long-run behavior of an optimal solution  $(P^*(\cdot), k^*(\cdot))$  can be characterized completely, see, e.g., [Wag03]. Each optimal solution converges to an OSS, and depending on the parameters (4) can have  $I = 1, 2, 3$  CSS  $(\hat{P}, \hat{q})_i$ ,  $i = 1, \dots, I$ .<sup>2</sup> For simplicity omitting the non-generic case  $I = 2$ , if  $I = 1$  then the unique CSS is a globally stable OSS, while for  $I = 3$  two CSS are locally stable OSS, and the third is unstable. Here a OSS  $(\hat{P}, \hat{q})$  is called globally (locally) stable if for each  $P(0)$  (in a neighborhood of  $\hat{P}$ ) the associated optimal path converges to  $(\hat{P}, \hat{q})$ ; see [KW10, Kis11] for a detailed discussion.

Setting  $u := (P, q)$  and letting  $\hat{u}$  be a steady state of (4), the problem now is to compute a path, or “connecting orbit”, with  $P(0) = P_0$  and  $\lim_{t \rightarrow \infty} u(t) = \hat{u}$ . One standard approach, see, e.g. [LK80, DCF<sup>+</sup>97, BPS01] and in particular [GCF<sup>+</sup>08, Chapter 7], is to treat (4) on a finite time interval  $[0, T]$  and to require  $u(T) \in W_s(\hat{u})$ , where  $W_s(\hat{u})$  is the local stable manifold of  $\hat{u}$ . In practice we approximate  $W_s(\hat{u})$  by the stable eigenspace  $E_s(\hat{u})$ , and thus require

$$u(T) \in E_s(\hat{u}) \text{ and close to } \hat{u}. \quad (8)$$

To obtain a well defined two point boundary value problem we then need  $\dim E_s(\hat{u}) = 1$ .

More generally, if the state variable is an  $n$ -dimensional vector and thus the canonical system is a system of  $2n$  ODEs, for arbitrary  $P_0$  we need that  $\hat{u}$  has the saddle point property, defined as follows.

**Definition 2.2** (Saddle Point Property). A CSS  $\hat{u} \in \mathbb{R}^{2n}$  with

$$n_s := \dim E_s(\hat{u}) = n \quad (9)$$

is called a CSS with the saddle point property (SPP). The number  $d(\hat{u}) := n_s - n$  is called the defect of  $\hat{u}$ , and a CSS with defect  $\hat{u} < 0$  is called defective.

For ODE problems like (4), given  $\hat{u}$  with the SPP, and some initial state  $P_0$ , canonical paths connecting  $P_0$  and  $\hat{u}$  can now be computed using, e.g., **OCMat**. We now generalize this to distributed problems, and thus in §3 explain further details on that level.

## 2.2 The shallow lake model with diffusion

Following [BX08] we consider the shallow lake model with diffusion in a domain  $\Omega \subset \mathbb{R}^d$ ,  $d = 1, 2$ , i.e.,

$$V(P_0(\cdot)) := \max_{k(\cdot, \cdot)} J(P_0(\cdot), k(\cdot, \cdot)), \quad J(P_0(\cdot), k(\cdot, \cdot)) := \int_0^\infty e^{-rt} J_{ca}(P(t), k(t)) dt, \quad (10a)$$

<sup>2</sup> cf., e.g., the FCSS branches in Fig. 1 for our specific parameter choice.

$$\text{where } J_{ca}(P(\cdot, t), k(\cdot, t)) = \frac{1}{|\Omega|} \int_{\Omega} J_c(P(x, t), k(x, t)) dx \quad (J_c(P, k) = \ln k - \gamma P^2 \text{ as before}) \quad (10b)$$

is the spatially averaged current value objective function, and  $P$  fulfills the initial boundary value problem

$$\partial_t P(x, t) = k(x, t) - bP(x, t) + \frac{P(x, t)^2}{1 + P(x, t)^2} + D\Delta P(x, t), \quad (10c)$$

$$\partial_{\nu} P(x, t)|_{\partial\Omega} = 0, \quad P(x, t)|_{t=0} = P_0(x), \quad x \in \Omega \subset \mathbb{R}^d, \quad (10d)$$

where  $\Delta = \partial_{x_1}^2 + \dots + \partial_{x_d}^2$ , and  $\nu$  is the outer normal of  $\Omega$ . We normalize  $J_{ca}$  by the domain size  $|\Omega|$  for easy comparison between the 0D, 1D, and 2D cases, and, more generally, between different domains. We mostly focus on  $\Omega = (-L, L)$  a real interval, but also give an outlook to 2D. In 2D the model is somewhat less intuitive, as a controlled phosphate dumping in the “middle” of the lake from farming appears difficult to motivate, and thus in 2D we rather think of (10) as a general pollution model. Instead of the periodic BC in 1D in [BX08] we require Neumann (zero flux) boundary conditions (BC), which from a modeling point of view we find more natural.

Introducing the costate  $q : \Omega \times (0, \infty) \rightarrow \mathbb{R}^N$  and the (local current value) Hamiltonian

$$\mathcal{H} = \mathcal{H}(P, q, k) = J_c(v, k) + q[k - bP + \frac{P^2}{1 + P^2} + D\Delta P], \quad (11)$$

by Pontryagin’s Maximum Principle for  $\tilde{\mathcal{H}} = \int_0^{\infty} e^{-rt} \overline{\mathcal{H}}(t) dt$  with the spatial integral

$$\overline{\mathcal{H}}(t) = \int_{\Omega} \mathcal{H}(P(x, t), p(x, t), k(x, t)) dx, \quad (12)$$

the canonical system for (10) becomes

$$\partial_t P(x, t) = [\partial_q H](x, t) = k(x, t) - bP(x, t) + \frac{P(x, t)^2}{1 + P(x, t)^2} + D\Delta P(x, t), \quad (13a)$$

$$\partial_t q(x, t) = r q(x, t) - [\partial_P H](x, t) = 2\gamma P(x, t) + q(x, t) \left( r + b - \frac{2P(x, t)}{(1 + P(x, t)^2)^2} \right) - D\Delta q(x, t), \quad (13b)$$

$$\partial_{\nu} P(x, t)|_{\partial\Omega} = 0, \quad \partial_{\nu} q(x, t)|_{\partial\Omega} = 0, \quad P(x, t)|_{t=0} = P_0(x), \quad x \in \Omega, \quad (13c)$$

where  $k = \operatorname{argmax}_{\tilde{k}} \mathcal{H}(P, q, \tilde{k})$ , which similar to (6) is obtained from

$$\partial_k \mathcal{H}(P, q, k) = 0 \quad \Leftrightarrow \quad k(x, t) = -\frac{1}{q(x, t)} \quad (13d)$$

The costate  $q$  also fulfills zero flux BC, and derivatives like  $\partial_P \mathcal{H}$  etc are taken variationally, i.e., for  $\overline{\mathcal{H}}$ . For instance, for  $\Phi(P, q) := q\Delta P$  we have  $\overline{\Phi}(P, q) = \int_{\Omega} q\Delta P dx = \int_{\Omega} (\Delta q)P dx$  by Gauß’ theorem, hence  $\delta_P \overline{\Phi}(P, q)[h] = \int_{\Omega} (\Delta q)h dx$ , and by the Riesz representation theorem we identify  $\delta_P \overline{\Phi}(P, q)$  and hence  $\partial_P \overline{\Phi}(P, q)$  with the multiplier  $\Delta q$ .

Finally, we have the limiting intertemporal transversality condition (see Remark 2.4 below)

$$\lim_{t \rightarrow \infty} e^{-rt} \int_{\Omega} q(x, t) P(x, t) dx = 0. \quad (14)$$

Analogous to Def. 2.1 we define

**Definition 2.3.** Let  $(P^*(\cdot, \cdot), k^*(\cdot, \cdot, P_0))$  be an optimal solution of problem (10), i.e. for every admissible  $k(\cdot, \cdot)$  and associated  $P(\cdot, \cdot)$  we have

$$J(P_0, k(\cdot, \cdot)) \leq J(P_0, k^*(\cdot, \cdot, P_0)) = V(P_0).$$

Then  $k^*(\cdot, \cdot, P_0)$  is called a (distributed) optimal control,  $P^*(\cdot, \cdot)$  is called the associated distributed optimal (state) path, and

$$\partial_t P(x, t) = k^*(x, t, P_0(x)) - bP(x, t) + \frac{P(x, t)^2}{1 + P(x, t)^2} + D\Delta P(x, t), \quad \partial_\nu P(x, t)|_{\partial\Omega} = 0 \quad (15)$$

is called the optimal PDE. Again with a slight abuse of notation,  $(P^*, k^*)$  is also called an optimal path, and an optimal stationary solution  $(\hat{P}(\cdot), \hat{k}(\cdot))$  of (13) is called an OSS (optimal steady state). If  $\hat{P}(\cdot) \equiv \hat{P}$  then the optimal steady state is called a FOSS (flat optimal steady state), otherwise it is called a POSS (patterned optimal steady state).

For a CSS  $\hat{u}(\cdot)$  we additionally introduce the acronyms *FCSS* for a flat canonical steady state, i.e.  $\hat{u}(\cdot) \equiv \hat{u}$ , and *PCSS* (patterned canonical steady state) otherwise. Obviously, the FCSS correspond precisely to the 0D CSS from §2.1. It was already indicated in [BX08] that (13) can additionally have PCSS arising from Turing like bifurcations. Thus, we first calculate bifurcation diagrams for (13), in 1D and 2D, recovering the up to 3 branches of FCSS from §2.1, and many branches of PCSS. Next, analogous to the 0D case, we expect a solution of (10) to converge to some CSS. Thus, we only consider solutions  $u(\cdot, \cdot)$  of (13) with  $\lim_{t \rightarrow \infty} u(\cdot, t) = \hat{u}(\cdot)$ , where  $\hat{u}(\cdot)$  is a CSS. For  $\hat{u}$  we then also need a version of the SPP. However,  $E_s(\hat{u})$  (and  $W_s(\hat{u})$ ) and  $E_u(\hat{u})$  (and  $W_u(\hat{u})$ ) are infinite dimensional. We circumvent this problem by requiring (8) and the saddle point property after a spatial discretization, which turns (13) into a (very large) systems of ODEs again. See App. A for further discussion.

**Remark 2.4.** (a) A strict mathematical proof of Pontryagin’s Maximum Principle for diffusion processes over an infinite time horizon is still missing, specifically for the transversality condition (14), which also in [BX08] is discussed only on a heuristic base. Thus, at the moment we apply Pontryagin’s Maximum Principle in an ad hoc sense. We specifically assume, based on the results for the 0D shallow lake model, that canonical paths converge to CSS, and therefore make no use of the “critical” transversality condition (14). In any case, a particular feature of the canonical system for diffusion processes is the anti-diffusion in the co-states, cf. (13b), which makes the canonical system ill-posed as an initial value problem.

(b) For background on OC in a PDE setting see also for instance [Trö10] and the references therein, or specifically [RZ99a, RZ99b, DHM12, ACKLT13] and [AAC11, Chapter5] for Pontryagin’s Maximum Principle for OC problems for semilinear parabolic state evolutions. However, these works are in a finite time horizon setting, and often the objective function is linear in the control and there are control constraints, e.g.,  $k(x, t) \in K$  with some bounded interval  $K$ . Therefore  $k$  is not obtained from the analogue of (13d), but rather takes the values from  $\partial K$ , which is usually called bang–bang control. In, e.g., [Neu03] and [DL09], stationary spatial OC problems for a fishery model with (active) control constraints are considered, including numerical simulations, which correspond to our calculation of canonical steady states for our SLOC model. Here we do not (yet) consider explicit control or state constraints, and have an objective function strictly concave in the control, and thus we have a rather different setting than the above works.

(c) We summarize that we do not aim at new theoretical results, but rather consider (13) after a spatial discretization as a (large) ODE problem, to which we apply the “connecting orbit method”. Importantly, this means that we take a broader perspective than aiming at computing just one optimal control, given an initial condition  $P_0$ , which without further information is an ill-posed problem anyway. Instead, our method aims to give a somewhat global picture by identifying the pertinent CSS and their respective domains of attraction. ]



### 3 Numerical algorithm, and results

The general idea is to use a method of lines discretization of (13), i.e., to approximate

$$u(x, t) := (P(x, t), q(x, t)) = \sum_{i=1}^{2n} u_i(t) \phi_i(x), \quad (16)$$

where  $(\phi_i)_{i=1, \dots, 2n}$  spans a subspace  $X_n$  of the phase space  $X$  of (13), e.g., here  $X = [H^1(\Omega)]^2$ , and  $(u_i, u_{n+i})$ ,  $i = 1, \dots, n$ , are the expansion coefficients of  $P, q$ , respectively. This converts (13) into a (high dimensional) ODE

$$\dot{u}(t) = -G(u(t)), \quad u_i(0) = u_{0,i}, \quad i = 1, \dots, n, \quad (17a)$$

for the coefficient vector  $u = (u_i)_{i=1, \dots, 2n}$ , where we have initial data for exactly half of the expansion coefficients. We choose a truncation time  $T$  and augment (17a) with the approximate transversality condition

$$u(T) \in E_s(\hat{u}), \quad \text{and } \|u(T) - \hat{u}\| \text{ small}, \quad (17b)$$

where  $\hat{u}$  is a steady state of (17a), and  $E_s(\hat{u})$  is spanned by the eigenvectors of  $-\partial_u G$  belonging to eigenvalues with negative real parts. As in 0D we then need the SPP, i.e.

$$\dim E_s(\hat{u}) = \dim E_u(\hat{u}), \quad (18)$$

to chose an arbitrary initial point in the state space. For a discussion and possible extension of the SPP to PDEs see App. A.

Arguably, the simplest discretization for (16), at least in 1D, is a finite difference (FD) scheme, which has the advantage that we can directly use `OCMat` for (17a), (17b), see [Gra15]. However, here we opt for a FEM ansatz for (16), using the setting of `pde2path` [UWR14, DRUW14] for two reasons:

1. We want to consider (10) and hence (13) also on general 2D domains, and for more general models where the state variables may be vector valued functions already, see §4, again in 1D or 2D. In all these cases, FD and the coding of the respective spatially discrete systems may become rather inconvenient, while `pde2path` provides convenient interfaces precisely for such systems. Moreover, for more complicated systems adaptive meshes may become important, which are more easily handled in a FEM discretization, and are already an integral part of `pde2path`.
2. As explained above, the canonical system may have many stationary states; it is thus desirable to use a continuation and bifurcation package to conveniently find CSS. The goal then is to “seamlessly” link the setting of `pde2path` for stationary problems with BVP solvers for (17a).

On the other hand, a drawback of spatial FEM discretizations is that the associated evolutionary problems have the natural form

$$M\dot{u}(t) = -Ku(t) + MF(u(t)) =: -G(u(t)), \quad (19)$$

where  $u$  corresponds to the nodal values,  $M, K \in \mathbb{R}^{2n \times 2n}$  are called the mass matrix and the stiffness matrix, respectively, and  $F : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$  is the nonlinearity. Thus,  $M$  and  $K$  are large but sparse; the “-” signs in (19) comes from the convention that `pde2path` discretizes  $-\Delta$  as  $K$  (positive definite). The occurrence of  $M$  on the left hand side of (19) means that it is not of the form (17a), and creates problems for the usage of standard BVP solvers. Of course,  $M$  is non-singular, and hence (19) can be rewritten as

$$\dot{u} = -M^{-1}Ku + F(u), \quad (20)$$

where for speed we can pre-calculate  $M^{-1}K$ . However,  $M^{-1}$  is no longer sparse, and already for intermediate  $n$  ( $n > 1000$ , say) this results in slow computations and in particular memory problems

when using standard BVP solvers, which sort the Jacobian  $-M^{-1}K + \partial_u F$  from each time-slice  $t_0, \dots, t_m$  into a big Jacobian for the BVP problem. This can be alleviated by providing an approximate Jacobian  $\tilde{J} = -A + \partial_u F$ , where  $A$  approximates  $M^{-1}K$  via lumping, i.e. we drop entries from  $M^{-1}K$  below a certain size  $\delta$ . Of course, there is a trade off between accuracy of  $\tilde{J}$  and the number of its nonzeros.

We mainly experimented with the `Matlab` solvers `bvp4c` and similar, for instance the adaptations of `bvp4c` already implemented in `OCMat`, and the solver TOM [MS02, MST09]<sup>3</sup>. It turned out that TOM worked best in the “lumped” setting. Moreover, TOM was easy to modify in an ad hoc way to handle  $M$  on the left hand side, and a new official release of TOM is scheduled that also uses  $M$  [Maz15]. For speedup it is advisable to avoid numerical differentiation and hence to pass a Jacobian function `J=fjac(t,u)` to TOM. This is generically very easy as `pde2path` in most cases provides a fast and easy way to assemble  $J$ . See [Uec15b] for implementation details.

### 3.1 The algorithm for the computation of a path to a CSS satisfying the SPP

To calculate canonical paths from a given state  $P_0$  that connect to some CSS  $\hat{u}$  with the SPP we want to solve the two-point BVP

$$M\dot{u}(t) = -G(u(t)), \quad t \in (0, T) \quad (21a)$$

$$P_i(0) = P_{0,i}, \quad i = 1, \dots, n, \quad (n \text{ left BC}), \quad (21b)$$

$$\Psi(u(T) - \hat{u}) = 0 \in \mathbb{R}^n \quad (n \text{ right BC}), \quad (21c)$$

where  $\Psi \in \mathbb{R}^{n \times 2n}$  encodes the projection onto the unstable eigenspace, i.e.  $\Psi(u - \hat{u}) = 0$  for  $u \in E_s(\hat{u})$ , and where  $T$  is the chosen truncation time. The calculation of  $\Psi$  at startup, which for large  $n$  turns out to be one of the bottlenecks of the algorithm, also gives a lower bound for the time scale  $T$  via  $T \geq \frac{1}{-\text{Re } \mu_1}$ , where  $\mu_1$  is the eigenvalue with largest negative real part, i.e., gives the slowest direction of the stable eigenspace of  $\hat{u}$ . In our simulations we typically use  $T$  between 50 and 100.

In general, a BVP solver needs a good initial guess of  $t \mapsto u(t)$  to solve problem (21). Therefore we embed problem (21) into a family of problems replacing (21b) by

$$P(0) = \alpha P_0 + (1 - \alpha) \hat{P}, \quad \alpha \in [0, 1], \quad (21d)$$

where we assume that for some  $\alpha$  the solution is known: this holds for instance for  $\alpha = 0$  with the trivial solution  $u \equiv \hat{u}$ . We may then gradually increase  $\alpha$ , using the last solution as the new initial guess. This is implemented in the algorithm summarized in Table 1.

There are more sophisticated variants of the simple continuation in Step 2 of Table 1 (some of which are implemented in `OCMat`), but the simple version in general works well for the problems we considered. Nevertheless, it may be that no solution of (21a), (21c) and (21d) is found for  $\alpha > \alpha_0$  for some  $\alpha_0 < 1$ , i.e., that the continuation to the intended initial point fails. In that case usually the BVP problem undergoes a fold bifurcation. We then use an adapted continuation step 2' that allows us to continue solutions around the fold.

**Remark 3.1.** (a) For some applications it is useful to rescale the time  $t = T\tau$  and hence consider  $M\dot{u}(\tau) = TG(u(\tau))$  on the normalized time interval  $\tau \in [0, 1]$ , which turns the truncation time  $T$  into a free parameter. This is for instance implemented in `OCMat`, but for simplicity not used here.

(b) Similarly to the normalized normalized objective value  $J_{ca}$  in (10b), in the bifurcation diagrams we use the normalized  $L^2$  norm for comparison between different domains and space dimensions, i.e., henceforth,  $\|P\|_2 := \|P\|_{L^2}/\sqrt{|\Omega|}$ , and in the table in Fig. 1 we present averaged values, i.e.,

$$\langle P \rangle := \frac{1}{|\Omega|} \int_{\Omega} P(x) \, dx, \quad \langle k \rangle := \frac{1}{|\Omega|} \int_{\Omega} k(x) \, dx. \quad (22)$$

<sup>3</sup>see also <http://www.dm.uniba.it/~mazzia/bvp/index.html>



- 
- Step 0 (selection of  $\hat{u}$  and implementation of (21c)). Given  $\hat{u}$  we solve the generalized adjoint EVP  $\partial_u G(\hat{u})^T \Phi = \Lambda M \Phi$  for the eigenvalues  $\Lambda$  and (adjoint) eigenvectors  $\Phi$ , which also gives the defect  $d(\hat{u})$ . If  $d(\hat{u}) = 0$ , then from  $\Phi \in \mathbb{C}^{2n \times 2n}$  we generate a real base of  $E_u(\hat{u})$  which we sort into the matrix  $\Psi \in \mathbb{R}^{n \times 2n}$ .
- Step 1 (selection of initial mesh and initial guess). To start the BVP solver we choose the initial guess  $u(t) \equiv \hat{u}$  on a suitable initial grid  $0 = t_0 < t_1 < \dots < t_m = T$ . Typically, we choose  $m = 20$  at startup, and afterwards TOM uses its own mesh-adaption strategy.
- Step 2 (solution and continuation). Using (21d) we try to increase  $\alpha$  in small steps  $\delta$  to  $\alpha = 1$ , in each step using the previous solution as the new initial guess, often trying  $\delta = 1/4$ . After thus having computed the first two solutions we may use a secant predictor for the subsequent steps.
- Step 2' (arclength continuation). If the continuation fails for  $\alpha > \alpha_0$  with  $\alpha_0 < 1$ , then we use a pseudo-arclength continuation for a modified BVP, letting  $\alpha$  be a free parameter.
- 

Table 1: The continuation-algorithm **iscont** (Initial State Continuation); Steps 0,1 are preparatory, Step 2 or 2' is repeated. See [Uec15b] for implementation details, and for remarks on performance.

To take the finite truncation time  $T$  into account we let

$$\tilde{J}(k(\cdot), T) := J(P_0(\cdot), k(\cdot, \cdot)) + \frac{e^{-rT}}{r} J_{ca}(P(T), k(T)). \quad (23)$$

Obviously, for  $T \gg \frac{1}{r}$  the last term can be made arbitrarily small, while for CSS it yields the exact (discounted) objective value. In the following we drop the tilde in (23), and write, e.g.,  $J_{\hat{u}}$  for the objective value of a CSS  $\hat{u}$ , and, e.g.,  $J_{P_1 \rightarrow \hat{u}}$  for the CS-path which goes from  $P_1$  to  $\hat{u}$ . ]

### 3.2 1D canonical steady states

Recall that first we use **pde2path** to study the steady state problem for (17a), i.e.,

$$0 = -\frac{1}{q(x)} - bP(x) + \frac{P(x)^2}{1 + P(x)^2} + D\Delta P(x), \quad (24a)$$

$$0 = 2cP(x) + q(x) \left( r + b - \frac{2P(x)}{(1 + P(x)^2)^2} \right) - D\Delta q(x), \quad (24b)$$

$$\partial_\nu P(x)|_{\partial\Omega} = 0, \quad \partial_\nu q(x)|_{\partial\Omega} = 0. \quad (24c)$$

In 1D we choose  $\Omega = (-L, L) \times (-\delta_y, \delta_y)$  with Neumann BC on all boundaries and small  $\delta_y$  such that we can use just two grid-points in  $y = x_2$ -direction and the solutions will be constant in  $y$ ; this we call a quasi 1D setup. The steady states of the canonical system for the 0D model (1) are FCSS of (24), and for easy reference we introduce the acronyms in Table 2. The FCSS are of course independent of the domain, but to search for PCSS bifurcating from FCSS, the domain size  $2L$  should be close to a multiple of  $2\pi/k_c$ , where  $k_c$  is the wave number of a Turing bifurcation. The parameters in (2), with  $b$  near 0.7, yield  $k_c \approx 0.44$  [BX08], and for simplicity we then choose  $L = 2\pi/0.44 \approx 14.28$ .

Continuing the FSI branch in  $b$  we find a number of Turing like bifurcations to PCSS, and follow four of these; see Fig. 1a,b for the bifurcation diagram(s), and (c) for example solutions<sup>4</sup>. On the branches p1,p2, and p3 there are secondary bifurcations, not further considered here. For the subsequent examples we focus on  $b = 0.75$  and  $b = 0.65$ , check the SPP (18) for all CSS and find it only to be

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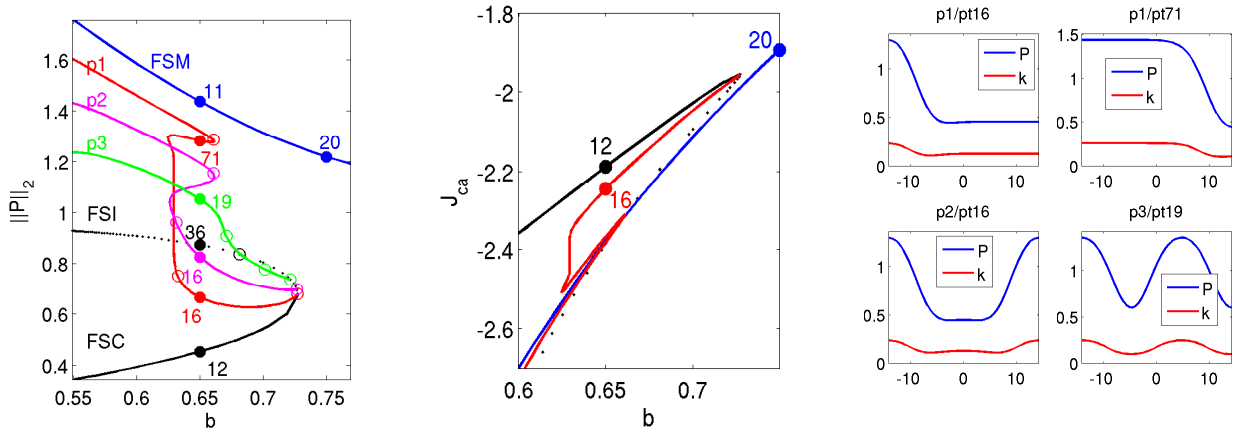
<sup>4</sup>The notation, e.g., p1/pt16 follows the **pde2path** scheme, e.g.: continuation step 16 on the branch p1 is stored in folder p1 and file pt16.mat.

name	description
FSM	Flat State Muddy, the upper FCSS branch with a high phosphor load $P$
FSI	Flat State Intermediate, the upper half of the second FCSS branch, intermediate $P$
FSC	Flat State Clean, the lower half of the second FCSS branch, low $P$

Table 2: Classification of the FCSS branches, see also Fig.1. The high  $P$  state is also called eutrophic, and our “muddy” refers to the fact that under eutrophic conditions there are a lot of algae and other organic matter in the lake, while under oligotrophic conditions (low  $P$ ) the water is much “cleaner”.

fulfilled for the FSM, for the FSC, and for some points on the p1 branch, e.g. at point 71 between the folds (see Fig. 1).

(a) BD of CSS, (normalized)  $L^2$  norm over  $b$  (b) BD, current values  $J_{c,a}$  (c) example CSS



(d) Characteristics of points in (a)-(c).

name	$\langle P \rangle$	$\langle k \rangle$	$J$	$d$	name	$\langle P \rangle$	$\langle k \rangle$	$J$	$d$
FSM/pt20	1.22	0.32	-63.11	0	p1/pt16	0.61	0.14	-74.83	-1
FSM/pt11	1.44	0.26	-79.28	0	p1/pt71	1.24	0.22	-78.93	0
FSI/pt36	0.87	0.13	-79.47	-5	p2/pt16	0.76	0.15	-76.70	-2
FSC/pt12	0.45	0.12	-72.95	0	p3/pt19	1.02	0.17	-79.48	-3

Figure 1: Basic bifurcation diagrams (a) and (b), example plots (c), and characteristic values of selected CSS (d). In (a), the blue and black lines represent the FCSS, and for instance the red line p1 contains patterned CSS with one “interface” between high and low  $P$ . The numbered points on all these lines correspond to selected solutions plotted in (c), and characterized in (d). The small circles in (a) denote bifurcation points. The values  $J_{ca}$  and  $J = J_{ca}/r$  of the CSS are all negative, but this is merely a question of offset.

### 3.3 1D canonical paths

For  $b = 0.75$ , the only CSS is the FSM (FSM/pt20). It has the SPP, we can reach it from an arbitrary initial state  $P_0$ , and thus it is a globally stable FOSS. Therefore, this regime is not very interesting, and we immediately turn to the case  $b = 0.65$  with multiple CSS.

For  $b = 0.65$  seven CSS are marked in Fig. 1a, and characterized in the table, where only three satisfy the SPP. These are the FSC (which has the maximal value among these CSS), the FSM, and

the PCSS `p1/pt71`, subsequently denoted as  $\hat{u}_{\text{PS}}$ . Next we numerically analyze which of these CSS belong to optimal paths.

### 3.3.1 PCSS not satisfying the SPP

From the analysis of non-distributed optimal control problems we know that steady states that do not satisfy the SPP can nevertheless be optimal. To illustrate that this is at least not typical in the SLOC model, we first compare the objective value of some (arbitrary chosen) CSS, e.g., the PCSS  $\hat{u}_{\text{PS}}(\cdot)$  `p3/pt19`, not satisfying the SPP, with that of the  $t$ -dependent canonical paths  $u_i(\cdot, \cdot)$  which connect to  $\hat{u}_i(\cdot)$ ,  $i \in \{\text{FSC}, \text{FSM}, \text{PS}\}$ . For the objective values we write  $J_{\text{PS}-}$  for the CSS, and, e.g.,  $J_{\text{PS}- \rightarrow \text{FSC}}$  for the canonical path which goes from  $P_{\text{PS}-}$  to  $\hat{u}_{\text{FSC}}$ . The optimal solution for  $P_0 = \hat{P}_{\text{PS}-}$  has to satisfy

$$V(\hat{P}_{\text{PS}-}) = \max\{J_{\text{PS}-}, J_{\hat{P}_{\text{PS}-} \rightarrow \text{FSC}}, J_{\hat{P}_{\text{PS}-} \rightarrow \text{FSM}}, J_{\hat{P}_{\text{PS}-} \rightarrow \text{PS}}\}. \quad (25)$$

The canonical paths are given in Fig. 2a–c, while (d) presents some norms along the path in (a), which show that and how fast  $u(t)$  (including the co-states  $q$ ) converges to  $\hat{u}$ . In all cases we find without problems canonical paths to both FCSS and the PCSS; in particular the path to FSM is rather quick.

For the objective values we find, up to 2 significant digits,

$$J_{\text{PS}-} = -79.48 < J_{\text{PS}- \rightarrow \text{FSC}} = -78.24 < J_{\text{PS}- \rightarrow \text{PS}} = -78.19 < J_{\text{PS}- \rightarrow \text{FSM}} = -77.5. \quad (26)$$

Thus, the optimal path is the one converging to  $\hat{u}_{\text{FSM}}$ . Repeating these steps for every PCSS not satisfying the SPP we find that these are always dominated by paths converging to one of the FCSS. Therefore, only  $\hat{u}_{\text{FSC}}$ ,  $\hat{u}_{\text{FSM}}$  and  $\hat{u}_{\text{PS}}$  remain as candidates for OSS.

Before we turn to determining OSS, we briefly discuss the canonical paths in Fig. 2. We focus on (a), but similar remarks apply to (b,c) as well. In (a), the initial  $P(\cdot, 0)$  is above the target  $\hat{P}_{\text{FSC}}$ , so naively we may expect that the control  $k$  should start below the target  $\hat{k}_{\text{FSC}}$  and slowly increase to  $\hat{k}_{\text{FSC}}$ . However, such a control would not be optimal. Instead,  $k$  is initially similar to  $\hat{k}_{\text{PS}-}$ , and in particular  $k(\cdot, 0)$  is large where  $P_0(\cdot)$  is already large. Only after a short transient  $k$  drops below  $\hat{k}_{\text{FSC}}$  and then behaves as expected.

At first sight, this startup behavior of  $k$  may appear rather counter-intuitive. However, the reason is that we do *not* want to drive the system to  $\hat{u}_{\text{FSC}}$  “as quickly as possible”, which essentially would amount to choosing  $k$  “as small as possible” at startup. Instead, we want to maximize  $J$ , and for this it pays off to have, for a short transient,  $k$  large near the maxima of  $P(\cdot, 0)$ .

To illustrate this point, in Fig. 2(e) we *choose* the naive control  $k(t) \equiv k_{\text{FSC}}$  for all  $t$  and numerically integrate the *initial value problem* (10c). While this does take us to  $\hat{u}_{\text{FSC}}$ , the first observation is that this needs a rather long time. Secondly, for the value of this solution we obtain  $J = -80.1$ , which is even worse than the starting CSS with  $J_{\text{PS}-} = -79.48$ .

### 3.3.2 Determining optimal steady states

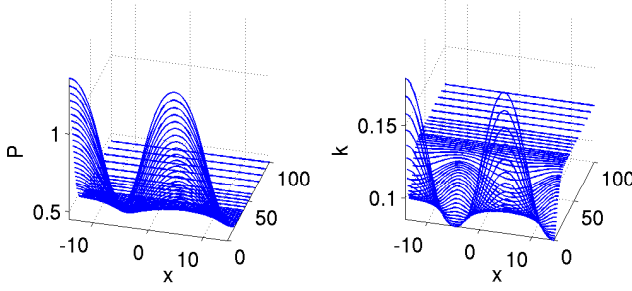
We return to the question whether one or more of the CSS at  $b = 0.65$  with the SPP from §3.3.1 are optimal, and proceed in three steps. First we search for a canonical path starting at  $\hat{P}_{\text{PS}}$  and connecting to  $\hat{u}_{\text{FSC}}$ . In the second step we repeat that for  $\hat{u}_{\text{FSM}}$ , and in the last step we check if both or only one of the FCSS are optimal.<sup>5</sup>

**Paths between  $\hat{P}_{\text{PS}}$  and  $\hat{u}_{\text{FSC}}$  – a Skiba candidate.** Using `iscont` to get a canonical path starting at  $\hat{P}_{\text{PS}}$  and converging to the FSC it turns out that the continuation (21d), i.e.,

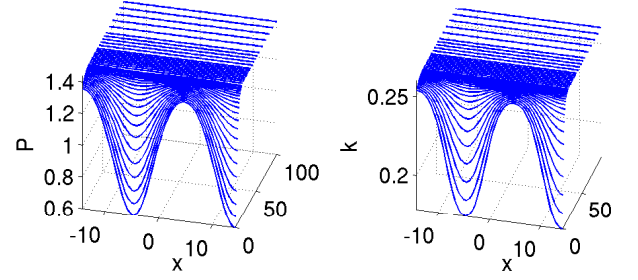
$$P_\alpha(0) := \alpha P_{\text{PS}} + (1 - \alpha) P_{\text{FSC}}, \quad (27)$$

<sup>5</sup>The second step reveals that the first step is superfluous, but this we do not know a priori.

(a) canonical path from p3/pt19 to FSC



(b) canonical path from p3/pt19 to FSM



(c) canonical path from p3/pt19 to PS

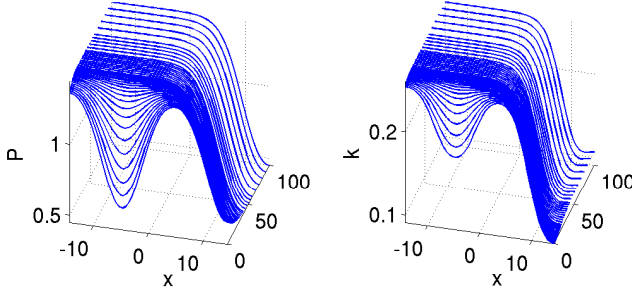
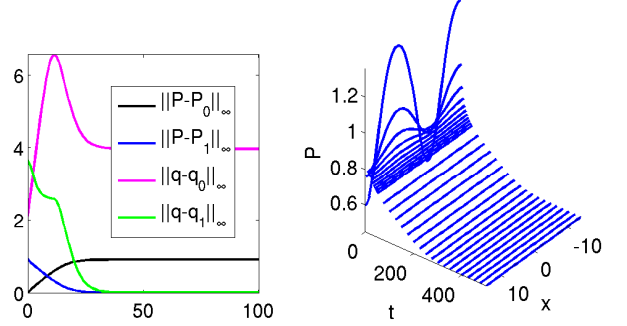
(d) diagnostics for a) (e)  $P$  for a naive control

Figure 2: Canonical paths from the (state values of) PCSS<sup>-</sup> p3/pt19 to FSC (a), FSM (b), and PS (c) at  $b = 0.65$ , and typical path diagnostics (d). For comparison, (e) shows the solution  $P$  of the initial value problem (10c) with  $P(0)$  as in (a) and the externally chosen control  $k(t) \equiv k_{\text{FSC}}$  for all  $t$ .

yields a fold around  $\alpha \approx 0.6$ , see the blue curve in Fig. 3a), and that no canonical path connecting  $\hat{P}_{\text{PS}}$  to  $\hat{u}_{\text{FSC}}$  exists. Instead, multiple solutions that converge to  $\hat{u}_{\text{FSC}}$  exist for initial distributions of the form (21d) with  $\alpha \in [0.6, 0.71]$ ; two examples are shown in Fig. 3b, and their diagnostics in (c).

Similarly, trying to continue to a path that connects  $\hat{P}_{\text{FSC}}$  and  $\hat{u}_{\text{PS}}$  yields a fold (green curve in (a)), and no such path exists. However, the solutions returned during the continuation process allow us to determine and compare the respective objective values. This yields that there exists a specific initial distribution where the objective values are equal, given by the intersection of the green and blue curves in Fig. 3a. Thus, from an economic point of view both solutions are equal. This suggests that  $P_S$  is a Skiba or indifference threshold point (distribution)<sup>6</sup>, well known from non-distributed optimal control problems, see, e.g., [Wag03, KW10]. The paths  $u$  starting at  $P_S$  (red curve) are depicted in Fig. 3d:  $P(\cdot, 0)$  is the same for both solutions, but the controls  $k(\cdot, 0)$  are different. In any case, to assure that these solutions are optimal we have to prove that no other dominating solution exists. Thus in a last step we calculate the objective values of the paths converging to  $\hat{u}_{\text{FSM}}$ .

**From  $\hat{P}_{\text{PS}}$  to  $\hat{u}_{\text{FSM}}$ .** Here the continuation is successful and we find a path connecting  $\hat{P}_{\text{PS}}$  to  $\hat{u}_{\text{FSM}}$ . Comparing the objective values reveals that the PCSS is dominated by the solution converging to the FSM, see Fig. 3e and 3f. Thus, the PCSS is ruled out as an optimal steady state, and therefore we a posteriori identify  $P_S$  as only a Skiba *candidate* as it does *not* separate two optimal steady states.

**A Skiba manifold between  $\hat{P}_{\text{FSM}}$  and  $\hat{P}_{\text{FSC}}$ .** It is well known that in 0D the FSC and FSM are only locally stable with regions of attractions separated by a Skiba manifold (parametrized by, e.g.,  $b$ ) of homogeneous solutions, [KW10], see Fig. 3g for our case  $b = 0.65$ . Of course, this also yields a

<sup>6</sup>however, taking into account also the FSM solution, below we identify  $P_S$  as only a Skiba candidate

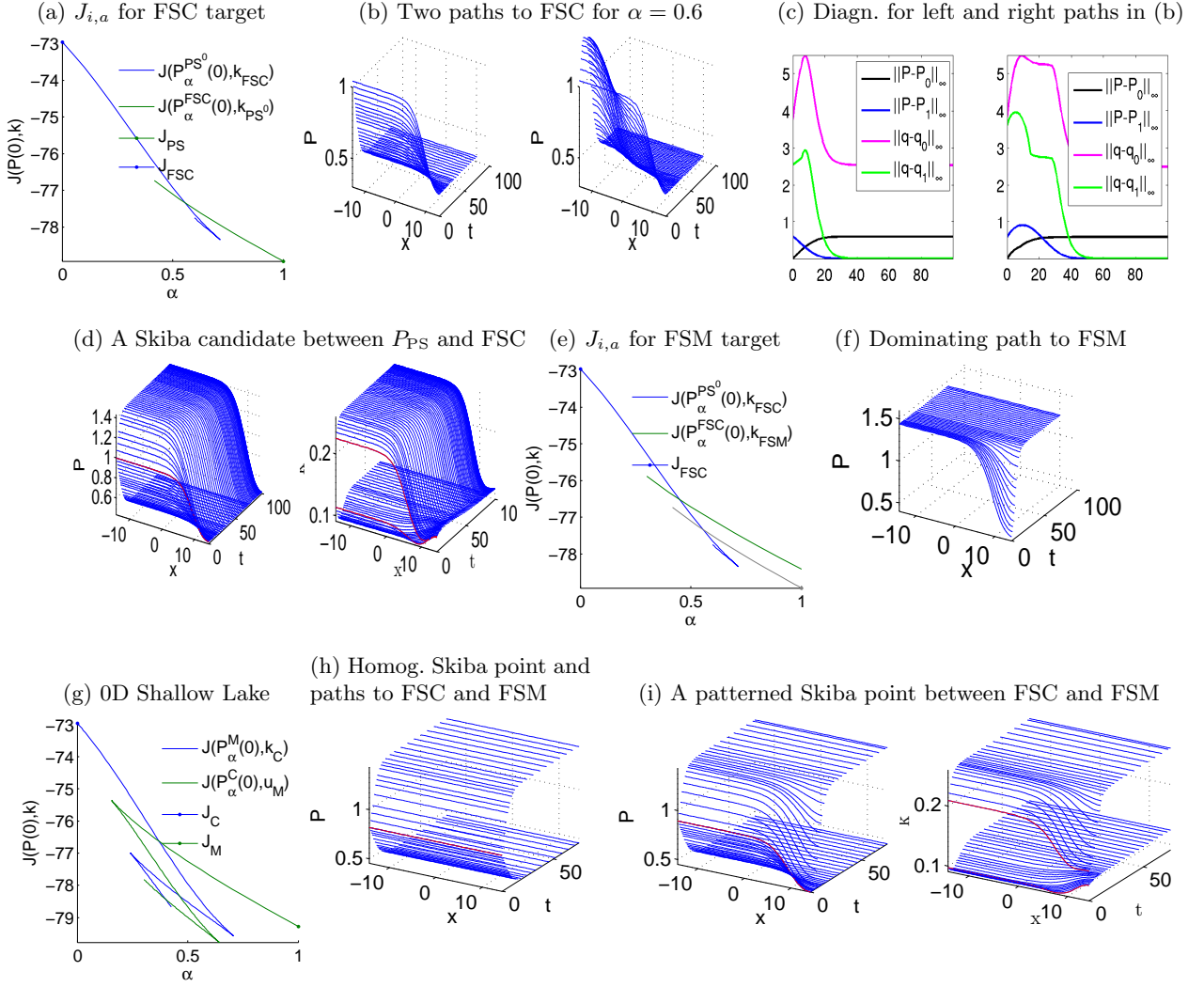


Figure 3: Canonical paths to various CSS for  $b = 0.65$ , and illustration of some Skiba points; see text for details.

homogeneous Skiba distribution in 1D, see Fig. 3h. More generally, we may expect the domains of attraction of the FSC and the FSM to be separated by an (in the continuum limit infinite dimensional) Skiba manifold  $M_S$ , for fixed  $b$ .

A continuation process, analogous to the non-distributed case, see [Gra12], could be used to approximate this manifold  $M_S$ . However, to find a non homogeneous example point on that manifold, here we can readily combine Fig. 3a and 3e, to find a Skiba distribution of the form

$$P_{\text{Skiba}} = \alpha \hat{P}_{\text{FSC}} + (1 - \alpha) \hat{P}_{\text{PS}}; \quad (28)$$

see Fig. 3i for paths to the FSC and the FSM yielding the same  $J = -76.3$ .

**Summary for 1D.** The picture that emerges is as follows: for  $b > b_{\text{fold}} \approx 0.727$  the FSM as the only CSS is the globally stable FOSS, while for  $b < b_{\text{fold}}$  there exist multiple CSS. Specifically for  $b = 0.65$ ,  $\hat{u}_{\text{FSC}}$ ,  $\hat{u}_{\text{FSM}}$  and one of the PCSS have the saddle point property, but only  $\hat{u}_{\text{FSC}}$  and  $\hat{u}_{\text{FSM}}$  are optimal, and in particular no POSS exists. The FOSS FSC and FSM are separated by a (presumably rather complicated) Skiba manifold  $M_S$ , and Fig. 3h and 3i show just two examples of points on  $M_S$ .

### 3.4 Outlook: 2D results

As a 2D example we consider (13) on the domain  $\Omega = (-L, L) \times (-L/2, L/2)$ ,  $L = 2\pi/0.44$  as before, with a rather coarse mesh of  $40 \times 20$  points, hence approximately 1600 DoF. The FCSS branches are of course the same as in 1D (or 0D), and again at the end of the FSI branch we find a number of Turing like bifurcations. In Fig. 4(a),(b) we only present the “new” patterned branches, i.e., those with a genuine  $x$  and  $y$  dependence.

(a) Two 2D PCSS branches

(b) some example plots

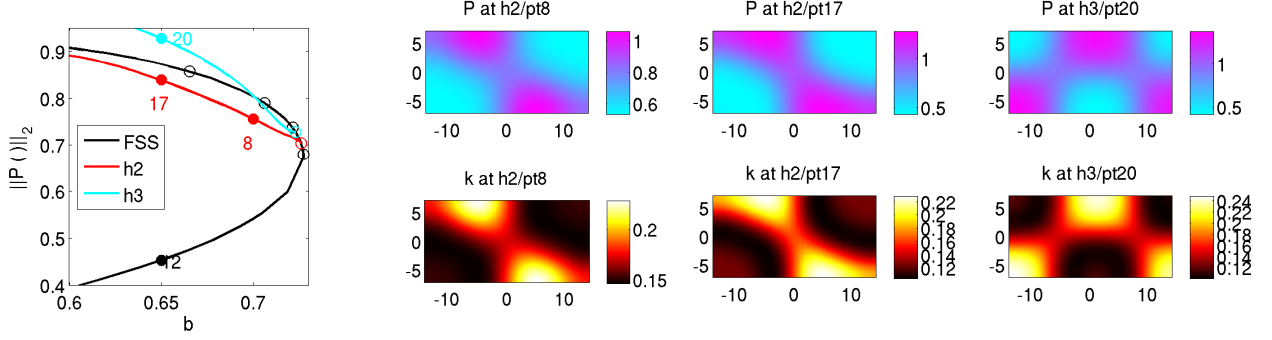


Figure 4: New patterned branches in 2D;  $(x, y) \in (-L, L) \times (-\frac{L}{2}, \frac{L}{2})$ .

These new bifurcating PCSS again do not fulfill the SPP. As an example for a canonical path, in Fig. 5 we present snapshots from a path from  $\hat{P}$  of the PCSS h2/pt17 to the FSC (see also [www.staff.uni-oldenburg.de/hannes.uecker/pde2path](http://www.staff.uni-oldenburg.de/hannes.uecker/pde2path) for the movie), which yields a higher  $J$  than the PCSS, i.e.,

$$J(\text{PCSS}) = -77.53 < J(\text{PCSS} \rightarrow \text{FSC}) = -76.23 < J(\text{FSC}) = -72.97. \quad (29)$$

Thus, this PCSS is not optimal, and neither is any other one we checked. Using the methods from §3.2 it is now of course also possible to find points with a genuine  $x$  and  $y$  dependence on the Skiba manifold separating FSC and FSM, but here we skip this presentation.

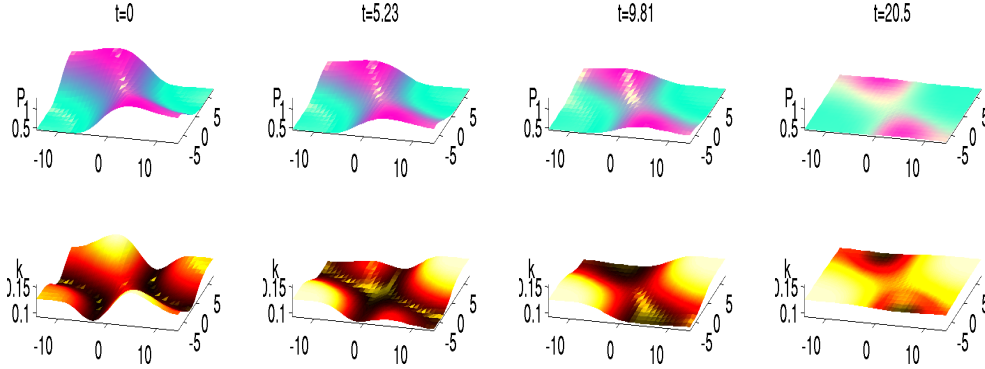


Figure 5: Solutions on the canonical path to FSC

The behavior and economic interpretation of the path from the PCSS to the FSC in Fig. 5 is rather similar to the convergence to the FSC in Fig. 2a. After a short transient the optimal strategy is to give a high phosphate load  $k$  where  $P$  is below the limit value  $\hat{P}_{\text{FSC}}$  (south-west and north-east corners of the domain), but initially there also is a high  $k$  at high  $P$  values (north-west and south-east corners).



## 4 Discussion

We have presented a numerical framework to treat infinite time horizon spatially distributed optimal control problems. First we derive the canonical PDE systems, which we then discretize in space and thus approximate by large systems of ODEs. For these we can resort to the theory and experience with non-distributed optimal control problems. Thus our results are intrinsically numerical; however, we believe that they can help to develop the theoretical concepts for distributed optimal control problems, following Oliver Heavisides’ saying “*Mathematics is an experimental science, and definitions do not come first, but later on.*”

From the economic point of view, the computation of canonical paths to the FOSS yields nontrivial and interesting results. Even more interesting would be locally stable POSS, but there is strong evidence that these do not exist for the shallow lake model (10), at least in the parameter regimes we considered so far<sup>7</sup>. On the other hand, in [Uec15a] we use our method to study the vegetation system from [BX10], and find that POSS dominate in large parameter regimes. We believe that the same happens in many other important systems, and a number of further investigations in this direction are under way. Natural candidates, i.e., systems with natural objective functions and controls, are related vegetation systems as in [SZvHM01, ZKY<sup>+</sup>13], fishery models as in [Neu03, Gra12], or “crimo-taxis” systems as in [SBB10].

## A SPP for PDEs

In this appendix we discuss the SPP (Def. 2.2) in a somewhat more general situation, tailored to canonical systems coming from spatial discretizations of PDEs. Let  $\hat{u} = (\hat{p}, \hat{q}) \in \mathbb{R}^{2N}$  be a stationary state of a (non-distributed) canonical system of the form

$$\frac{d}{dt} \begin{pmatrix} p \\ q \end{pmatrix} = F(p, q) := \begin{pmatrix} f(p, q) \\ rq - H_p(p, q) \end{pmatrix}, \quad (30)$$

where  $f = H_q$ , and let  $J = D_u F(\hat{u})$  be the Jacobian at  $\hat{u}$ . In [GCF<sup>+</sup>08, Thm 7.10] it is explained that the eigenvalues of  $J$  are symmetric around  $r/2$ , i.e., that there exist  $N$  complex numbers  $\xi_i$  such that

$$\sigma(J) = \left\{ \frac{r}{2} \pm \xi_i : i = 1, \dots, N \right\}. \quad (31)$$

In detail, since  $\det(J - \xi) = \det(J_r - (\xi - \frac{r}{2}))$  where

$$J_r := J - \frac{r}{2} = \begin{pmatrix} H_{pq} - \frac{r}{2} & H_{qq} \\ -H_{pp} & -H_{pq} + \frac{r}{2} \end{pmatrix}, \quad (32)$$

we have that  $\frac{r}{2} + \xi_i \in \mathbb{C}$  is an eigenvalue of  $J$  if and only if  $\xi_i$  is an eigenvalue of  $J_r$ . But  $J_r$  has the structure  $\begin{pmatrix} A & B \\ C & -A \end{pmatrix}$  with symmetric matrices  $B, C \in \mathbb{R}^{N \times N}$ , and as a consequence the eigenvalues of  $J_r$  are  $\xi_i = \pm \sqrt{\tilde{\xi}_i}$ ,  $i = 1, \dots, N$ .

Now consider the distributed canonical system

$$\partial_t \begin{pmatrix} p(x, t) \\ q(x, t) \end{pmatrix} = F(p(x, t), q(x, t)) + \begin{pmatrix} D\Delta p(x, t) \\ -D\Delta q(x, t) \end{pmatrix}, \quad (33)$$

where  $D \in \mathbb{R}^{N \times N}$  is a diffusion matrix, i.e., positive definite. Let

$$\frac{d}{dt} u(t) = G(u(t)), \quad u \in \mathbb{R}^{2nN}, \quad (34)$$

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<sup>7</sup> see however “Scenario 2” in [Gra15] for some locally stable POSS

be the associated spatially discretized system with  $n$  spatial points, where  $u = (p(x_1), \dots, p(x_n), q(x_1), \dots, q(x_n)) \in \mathbb{R}^{2nN}$ , and let  $\hat{u} \in \mathbb{R}^{2nN}$  be a steady state of (34). Then  $J = D_u G(\hat{u})$  has the structure  $J = -K + J_{\text{local}}$ , where  $J_{\text{local}}$  has the block structure

$$J_{\text{local}} = \begin{pmatrix} H_{pq}^1 & 0 & \dots & 0 & H_{qq}^1 & 0 & \dots & 0 \\ 0 & H_{pq}^2 & \dots & 0 & 0 & H_{qq}^2 & \dots & 0 \\ \vdots & \vdots & \ddots & \dots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & H_{qq}^n & 0 & 0 & \dots & H_{qq}^n \\ -H_{pp}^1 & 0 & \dots & 0 & r - H_{qp}^1 & 0 & \dots & 0 \\ 0 & -H_{pp}^2 & \dots & 0 & 0 & r - H_{qp}^2 & \dots & 0 \\ \vdots & \vdots & \ddots & \dots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & -H_{pp}^n & 0 & 0 & \dots & r - H_{qp}^n \end{pmatrix}, \quad (35)$$

composed of local matrices  $H_{pq}^j := H_{pq}(x_j) := H_{pq}(p(x_j), q(x_j))$ ,  $H_{qq}^j, H_{pp}^j \in \mathbb{R}^{N \times N}$ , and  $K = \begin{pmatrix} L & 0 \\ 0 & -L \end{pmatrix}$  with  $L \in \mathbb{R}^{nN}$  coming from the discretization of  $D\Delta$ . The notation  $K$  of course reflects the FEM background of the present paper, but the same structure  $\begin{pmatrix} L & 0 \\ 0 & -L \end{pmatrix}$  occurs for any discretization, in any space dimension, and for any  $D$  not necessarily diagonal, i.e., containing cross diffusion.

It follows that again  $\frac{r}{2} + \xi_i$  is an eigenvalue of  $J$  if and only if  $\xi$  is an eigenvalue of  $J_r := J - \frac{r}{2}$ , where  $J_r$  has the structure

$$J_r = \begin{pmatrix} A & B \\ C & -A \end{pmatrix}, \text{ with symmetric } B, C \in \mathbb{R}^{nN}.$$

Applying [GCF<sup>+</sup>08, Lemma B.2, Lemma B.3] we obtain

**Theorem A.1.** *Let  $\hat{u}$  be a steady state of the spatially discretized distributed system (34), and let  $J$  be the associated Jacobian. Then there exist  $\xi_i \in \mathbb{C}$ ,  $i = 1, \dots, nN$ , such that*

$$\sigma(J) = \left\{ \frac{r}{2} \pm \xi_i : i = 1, \dots, nN \right\}. \quad (36)$$

As a consequence,  $\dim E_s(\hat{u}) \leq Nn$ , and the only candidates  $\hat{u}$  for right BC in (21c) are those with the SPP. As a corollary we find a property that, on the discretized level, is equivalent to the SPP.

**Corollary A.2.** *Let  $\hat{u} \in \mathbb{R}^{2nN}$  be an equilibrium of the spatially discretized distributed system (34) and  $r > 0$ . Then  $\hat{u}$  satisfies the SPP iff every eigenvalue  $\xi$  of the according Jacobian  $J(\hat{u})$  satisfies*

$$\|\operatorname{Re} \xi - \frac{r}{2}\| > \frac{r}{2}. \quad (37)$$

**Remark A.3.** Theorem A.1 is formulated on the discretized level, and one might ask how it ultimately relates to the PDE. As a first step one can ask: Let a steady state  $\hat{u} \in \mathbb{R}^{2nN}$  of (34) be an approximation of a PDE steady state  $(\hat{p}, \hat{q}) \in X$  for (33), with  $X \subset \{(p, q) : \Omega \rightarrow \mathbb{R}^{2N}\}$  some function space, e.g.,  $X = [H^1(\Omega)]^{2N}$ . If  $\tilde{u} \in \mathbb{R}^{2\tilde{n}N}$  is an approximation of  $(\hat{p}, \hat{q})$  on a finer mesh  $\tilde{n} > n$ , or just a different mesh, do we have

$$nN - \dim E_s(\hat{u}) = \tilde{n}N - \dim E_s(\tilde{u}) \quad ? \quad (38)$$

We do not want to go into the details here, but if  $E_c(\hat{u}) = \emptyset$ , i.e.,  $\sigma(J) \cap \{\operatorname{Re} \xi = 0\} = \emptyset$ , then (38) is true, for large enough  $n, \tilde{n}$ . Given some  $\hat{u}$ , this can be easily tested numerically, and it is also clear from an analytical point of view. Refining  $\hat{u}$  to  $\tilde{u}$  we essentially add high frequency modes to the FEM (or finite difference) mesh. These introduce the same number of additional eigenvalues at

large positive and negative  $\xi$  for the linearization  $\tilde{J}$ , because  $J_F(p, q) : X \rightarrow X$  is relatively compact with respect to the Laplacian, i.e., w.r.t.  $(p, q) \mapsto (D\Delta p, -D\Delta q)$ . On the other hand, the small eigenvalues  $\mu_i$ ,  $|\mu_i| < R$  for some fixed  $R$ , are only slightly perturbed, i.e.,  $|\mu_i - \tilde{\mu}_i| \leq C\|\hat{u}_* - \tilde{u}\|$ , where  $\hat{u}_*$  is suitably defined, for instance by interpolating  $\hat{u}$  to the mesh of  $\tilde{u}$ . But  $\|\hat{u}_* - \tilde{u}\| \rightarrow 0$  as  $n, \tilde{n} \rightarrow \infty$ , which yields (38).

To make this rigorous, we need to define appropriate function spaces and study the approximation properties of the spatial discretization. This is easy, as the stationary problem for (33) can be written as an elliptic system, and hence  $(p, q)$  is arbitrary smooth, but we omit the details here.

In fact, (37) can also be formulated on the PDE level and might therefore replace the SPP from Def. 2.2 for spatially distributed models. However, we also postpone an in depth analysis of this to future work.

## References

- [AAC11] S. Anița, V. Arnăutu, and V. Capasso. *An introduction to optimal control problems in life sciences and economics*. Birkhäuser/Springer, New York, 2011.
- [ACKLT13] S. Anița, V. Capasso, H. Kunze, and D. La Torre. Optimal control and long-run dynamics for a spatial economic growth model with physical capital accumulation and pollution diffusion. *Appl. Math. Lett.*, 26(8):908–912, 2013.
- [ADS14] N. Apreutesei, G. Dimitriu, and R. Strugariu. An optimal control problem for a two-prey and one-predator model with diffusion. *Comput. Math. Appl.*, 67(12):2127–2143, 2014.
- [BPS01] W.J. Beyn, Th. Pampel, and W. Semmler. Dynamic optimization and Skiba sets in economic examples. *Optimal Control Applications and Methods*, 22(5–6):251–280, 2001.
- [BX08] W.A. Brock and A. Xepapadeas. Diffusion-induced instability and pattern formation in infinite horizon recursive optimal control. *Journal of Economic Dynamics and Control*, 32(9):2745–2787, 2008.
- [BX10] W. Brock and A. Xepapadeas. Pattern formation, spatial externalities and regulation in coupled economic–ecological systems. *Journal of Environmental Economics and Management*, 59(2):149–164, 2010.
- [CB04] S.R. Carpenter and W.A. Brock. Spatial complexity, resilience and policy diversity: fishing on lake-rich landscapes. *Ecology and Society*, 9(1), 2004.
- [Cla90] C. W. Clark. *Mathematical bioeconomics*. John Wiley & Sons, Inc., New York, second edition, 1990. The optimal management of renewable resources.
- [DCF<sup>+</sup>97] E. Doedel, A. R. Champneys, Th. F. Fairgrieve, Y. A. Kuznetsov, Bj. Sandstede, and X. Wang. AUTO: Continuation and bifurcation software for ordinary differential equations (with HomCont). <http://cmvl.cs.concordia.ca/auto/>, 1997.
- [DHM12] W. Ding, V. Hryniv, and X. Mu. Optimal control applied to native–invasive species competition via a PDE model. *EJDE*, 2012(237):1–18, 2012.
- [DL09] W. Ding and S. Lenhart. Optimal harvesting of a spatially explicit fishery model. *Natural Resource Modeling*, 22(2):173–211, 2009.
- [DRUW14] T. Dohnal, J. Rademacher, H. Uecker, and D. Wetzel. pde2path 2.0. In H. Ecker, A. Steindl, and S. Jakubek, editors, *ENOC 2014 - Proceedings of 8th European Nonlinear Dynamics Conference*, ISBN: 978-3-200-03433-4, 2014.

- [GCF<sup>+</sup>08] D. Grass, J.P. Caulkins, G. Feichtinger, G. Tragler, and D.A. Behrens. *Optimal Control of Nonlinear Processes: With Applications in Drugs, Corruption, and Terror*. Springer Verlag, 2008.
- [Gra12] D. Grass. Numerical computation of the optimal vector field in a fishery model. *Journal of Economic Dynamics and Control*, 36(10):1626–1658, 2012.
- [Gra15] D. Grass. From 0D to 1D spatial models using OCMat. Technical report, ORCOS, 2015.
- [Kis11] T. Kiseleva. *Structural Analysis of Complex Ecological Economic Optimal Control Problems*. PhD thesis, University of Amsterdam, Center for Nonlinear Dynamics in Economics and Finance (CeNDEF), 2011.
- [KW10] T. Kiseleva and F.O.O. Wagener. Bifurcations of optimal vector fields in the shallow lake system. *Journal of Economic Dynamics and Control*, 34(5):825–843, 2010.
- [LK80] M. Lentini and H.B. Keller. Boundary value problems on semi-infinite intervals and their numerical solution. *SIAM Journal on Numerical Analysis*, 17(4):577–604, 1980.
- [LW07] S. Lenhart and J. Workman. *Optimal Control Applied to Biological Models*. Chapman Hall, 2007.
- [Maz15] F. Mazzia. Private communication, 2015.
- [MS02] F. Mazzia and I. Sgura. Numerical approximation of nonlinear BVPs by means of BVMs. *Applied Numerical Mathematics*, 42(1–3):337–352, 2002. Numerical Solution of Differential and Differential-Algebraic Equations, 4-9 September 2000, Halle, Germany.
- [MST09] F. Mazzia, A. Sestini, and D. Trigiante. The continuous extension of the B-spline linear multistep methods for BVPs on non-uniform meshes. *Applied Numerical Mathematics*, 59(3–4):723–738, 2009.
- [MXdZ03] K.G. Mäler, A. Xepapadeas, and A. de Zeeuw. The economics of shallow lakes. *Environmental and Resource Economics*, 26(4):603–624, 2003.
- [Neu03] M. G. Neubert. Marine reserves and optimal harvesting. *Ecology Letters*, 6(9):843–849, 2003.
- [PBGM62] L.S. Pontryagin, V.G. Boltyanskii, R.V. Gamkrelidze, and E.F. Mishchenko. *The Mathematical Theory of Optimal Processes*. Wiley-Interscience, New York, 1962.
- [RZ99a] J. P. Raymond and H. Zidani. Hamiltonian Pontryagin’s principles for control problems governed by semilinear parabolic equations. *Appl. Math. Optim.*, 39(2):143–177, 1999.
- [RZ99b] J. P. Raymond and H. Zidani. Pontryagin’s principle for time-optimal problems. *J. Optim. Theory Appl.*, 101(2):375–402, 1999.
- [SBB10] M. B. Short, A. L. Bertozzi, and P. J. Brantingham. Nonlinear patterns in urban crime: hotspots, bifurcations, and suppression. *SIAM J. Appl. Dyn. Syst.*, 9(2), 2010.
- [Sch98] M. Scheffer. *Ecology of Shallow Lakes*. Kluwer Academic Publishers, 1998.
- [SZvHM01] M. Shachak, Y. Zarmi, J. von Hardenberg, and E. Meron. Diversity of vegetation patterns and desertification. *PRL*, 87, 2001.
- [Trö10] Fredi Tröltzsch. *Optimal control of partial differential equations*, volume 112 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, 2010.

- [Uec15a] H. Uecker. Optimal control and spatial patterns in a semi arid grazing system. Preprint, 2015.
- [Uec15b] H. Uecker. The pde2path add-on library p2poc for solving o infinite time–horizon spatially distributed optimal control problems - Quickstart Guide. Preprint, 2015.
- [UWR14] H. Uecker, D. Wetzel, and J. Rademacher. pde2path – a Matlab package for continuation and bifurcation in 2D elliptic systems. *NMTMA*, 7:58–106, 2014.
- [Wag03] F.O.O. Wagener. Skiba points and heteroclinic bifurcations, with applications to the shallow lake system. *Journal of Economic Dynamics and Control*, 27(9):1533–1561, 2003.
- [ZKY<sup>+</sup>13] Y. Zelnik, S. Kinast, H. Yizhaq, G. Bel, and E. Meron. Regime shifts in models of dryland vegetation. *Philos. Trans. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci.*, 371(2004), 2013.